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No-core shell model for ^{48}Ca , ^{48}Sc and ^{48}Ti

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Abstract

We report the first no-core shell model results for ^{48}Ca , ^{48}Sc and ^{48}Ti with derived and modified two-body Hamiltonians. We use an oscillator basis with a limited $\hbar\Omega$ range around $45/A^{1/3} - 25/A^{2/3} = 10.5\text{MeV}$ and a limited model space up to $1\hbar\Omega$. No single-particle energies are used. We find that the charge dependence of the bulk binding energy of eight $A = 48$ nuclei is reasonably described with an effective Hamiltonian derived from the CD-Bonn interaction while there is an overall underbinding by about 0.4 MeV/nucleon . However, resulting spectra exhibit deficiencies that are anticipated due to: (1) basis space limitations and/or the absence of effective many-body interactions; and, (2) the absence of genuine three-nucleon interactions. We then introduce additive isospin-dependent central terms plus a tensor force to our Hamiltonian and achieve accurate binding energies and reasonable spectra for all three nuclei. The resulting no-core shell model opens a path for applications to the double-beta ($\beta\beta$) decay process.

I. INTRODUCTION

Motivated by the need for precision treatments of nuclear matrix elements involved in the double-beta ($\beta\beta$) decay process, we investigate the ab-initio no core shell model (NCSM) for the lightest case of such a decay, which involves the ^{48}Ca , ^{48}Sc and ^{48}Ti nuclei.

Previous efforts have addressed $A = 48$ nuclei with similar goals by solving the shell model of eight nucleons in the pf shell with a ^{40}Ca core. Chief among these efforts is the work of Caurier et al. [1] who made predictions for the $2\nu\beta\beta$ decay mode of ^{48}Ca . They carried out a full $0\hbar\Omega$ calculation for the nuclei involved in this decay, using a KB3 effective interaction [2]. Single-particle energies extracted from experiment were used to model the valence-core interactions. They obtained a satisfactory description of the spectroscopy (energy levels of positive parity, E2 and M1

transitions) when they used a factor of 0.77 to renormalize the NME of the Gamow-Teller (GT) operator $\sigma\tau_{\pm}$. This quenching factor accounts for possible missing nucleon correlations and/or non-nucleonic contributions.

Similar calculations have been performed using either slightly different parameters in the Hamiltonian [3] or more severely truncated model spaces [4], but the predicted half-lives differ from the experimental value by a factor 2-3. Such calculations have also been extended to the $0\nu\beta\beta$ decay mode of ^{48}Ca [5]. The authors used two NN interactions (KB3 and RVJB [6]) and performed calculations using both the full pf shell model space and another three truncated spaces. They concluded that in this case the results are not significantly dependent on the truncation as long as the 2p-2h correlations are included.

Caurier et al. [7] also performed a systematic calculation of the spectroscopic properties (positive parity energy levels, $B(E2)$, $M1$, quadrupole moments, GT strengths) of several $A = 48$ isotopes: ^{48}Ca , ^{48}Sc , ^{48}Ti , ^{48}V , ^{48}Cr and ^{48}Mn . The model space consisted again of 8-nucleons in the full pf shell and they used a minimally monopole modified realistic KB3 interaction along with experimental single particle energies. Their results reproduced well the existing data with very few parameters. The calculated GT strengths are in agreement with experiment using the standard quenching factor mentioned above and display a fine structure which indicates that fragmentation renders much of the GT strength unobservable.

Alternatively, in ref. [8] the authors performed a full pf shell model calculation of the $2\nu\beta\beta$ decay rate of ^{48}Ca using a Hamiltonian given as a set of 195 two-body NME. They examined how modifications in the Hamiltonian influence the value of the decay rate and concluded that with an appropriate change in the pairing interaction one may obtain satisfactory agreement with experiment without renormalizing the GT operators. In addition, they found that making the quadrupole force more attractive is equivalent with making the pairing weaker.

Other works performing a shell model calculation of the $2\nu\beta\beta$ NME emphasize the role of the nuclear shell structure, which gives rise to a concentration or fragmentation of the decay rate components over the intermediate states ([10]) and the important role of the spin-orbit term, compared with the other terms of a schematic potential that also included central and tensor terms ([11]).

Finally, we mention that more details on the capabilities of the Shell Model to describe complex manifestations of nuclear dynamics can be found in a recent review written by Caurier et al.([9]).

As an alternative approach, we investigate the NCSM for these $A = 48$ nuclei. This is the first time such calculations are reported for nuclei with $A \geq 17$. Our initial goal is to demonstrate the limited feasibility of such NCSM calculations in this region. We will display the current status of the NCSM and, with phenomenology, also demonstrate how far we still must go before addressing

fundamental processes such as $\beta\beta$ decay rates. Due to the considerable gap between present NCSM theory and the best fit results, we defer evaluations of decay rates to later efforts.

The main ingredients of our approach are the following:

- 1) We adopt the NCSM approach and approximate the full H_{eff} with a two-body cluster truncation. In solving the $A = 48$ systems, all nucleons are treated with the same two-body Hamiltonian derived from a realistic NN interaction including Coulomb interaction between proton pairs. There are no single particle energies involved and the eigenenergies are the total binding energies.
- 2) We work in a neutron-proton basis so full isospin mixing is allowed including isospin mixing arising from the bare NN interaction and those induced within H_{eff} itself.
- 3) For 48-Ca we evaluate both the positive (0hw) and negative parity (1hw) spectra.
- 4) Our solutions are free of spurious center of mass motion effects.
- 5) Our wavefunctions exactly obey the Ikeda sum rule [12].
- 6) We provide a baseline for further improvements to H_{eff} such as the inclusion of real and effective three-body forces.
- 7) We show that by introducing of a few phenomenological terms the description of both the BE/A and the low-lying spectra for all three nuclei improve considerably.

Of course the present work has a significant drawback. Due to the limited model space and the neglect of real and effective three-body interactions, we must resort to additive phenomenological terms to obtain high quality description of selected experimental data. The dependence on the parameters introduced, including the basis space parameters N_{max} and $\hbar\Omega$, as well as dependence on the forms and strengths of the additive potential terms, severely limit the predictive power of our present approach. On the other hand, the descriptions achieved with our initial choice of additive terms provides insight into the deficiencies of our current H_{eff} in the $0\hbar\Omega$ and $1\hbar\Omega$ model spaces.

The paper is organized as follows. In section 2 we give a brief description of the NCSM formalism. In section 3 we present our results and analysis and section 4 is devoted to conclusions and perspectives.

II. NO CORE SHELL MODEL (NCSM) FORMALISM

In order to take a step towards increased predictive power, we adapt the recently derived ab-initio NCSM as we will briefly outline here. However, due to computational limitations translating into model space limitations, we expect and find that the spectroscopic results differ significantly from experiment. Since previous investigations summarized above have indicated the importance of obtaining good spectroscopic descriptions in order to minimize uncertainties in predictions of

key experimental observables, we will introduce additive phenomenological corrections sufficient to fit experimental spectra.

A. Basic NCSM and Effective Hamiltonian

The NCSM [13]-[18] is based on an effective Hamiltonian derived from realistic “bare” interactions and acting within a finite Hilbert space. All A -nucleons are treated on an equal footing. The approach is demonstrably convergent to the exact result of the full (infinite) Hilbert space.

Initial investigations used two-body interactions [13] based on a G-matrix approach. Later, we implemented the Lee-Suzuki-Okamoto procedure [19, 20] to derive two-body and three-body effective interactions based on realistic NN and NNN interactions.

For pedagogical purposes, we outline the NCSM approach with NN interactions alone and point the reader to the literature for the extensions to include NNN interactions. We begin with the purely intrinsic Hamiltonian for the A -nucleon system, i.e.,

$$H_A = T_{\text{rel}} + \mathcal{V} = \frac{1}{A} \sum_{i < j}^A \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i < j=1}^A V_N(\vec{r}_i - \vec{r}_j) , \quad (1)$$

where m is the nucleon mass and $V_N(\vec{r}_i - \vec{r}_j)$, the NN interaction, with both strong and electromagnetic components. Note the absence of a phenomenological single-particle potential. We may use either coordinate-space NN potentials, such as the Argonne potentials [21] or momentum-space dependent NN potentials, such as the CD-Bonn [22] which we select for the present investigation.

Next, we add the center-of-mass HO Hamiltonian to the Hamiltonian (1) $H_{\text{CM}} = T_{\text{CM}} + U_{\text{CM}}$, where $U_{\text{CM}} = \frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = \frac{1}{A}\sum_{i=1}^A\vec{r}_i$. In the full Hilbert space the added H_{CM} term has no influence on the intrinsic properties. However, when we introduce our cluster approximation below, the added H_{CM} term facilitates convergence to exact results with increasing basis size. The modified Hamiltonian, with a pseudo-dependence on the HO frequency Ω , can be cast into the form

$$H_A^\Omega = H_A + H_{\text{CM}} = \sum_{i=1}^A \left[\frac{\vec{p}_i^2}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^2 \right] + \sum_{i < j=1}^A \left[V_N(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2 \right] . \quad (2)$$

In the spirit of Da Providencia and Shakin [23] and Lee, Suzuki and Okamoto [19, 20], we introduce a unitary transformation, which is able to accommodate the short-range two-body correlations in a nucleus, by choosing an antihermitian operator S , acting only on intrinsic coordinates, such that

$$\mathcal{H} = e^{-S} H_A^\Omega e^S . \quad (3)$$

In our approach, S is determined by the requirements that \mathcal{H} and H_A^Ω have the same symmetries and eigenspectra over the subspace \mathcal{K} of the full Hilbert space. In general, both S and the transformed

Hamiltonian are A -body operators. Our simplest, non-trivial approximation to \mathcal{H} is to develop a two-body ($a = 2$) effective Hamiltonian, where the upper bound of the summations “ A ” is replaced by “ a ”, but the coefficients remain unchanged. The next improvement is to develop a three-body effective Hamiltonian, ($a = 3$). This approach consists then of an approximation to a particular level of clustering with $a \leq A$.

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(a)} = \sum_{i=1}^A h_i + \frac{\binom{A}{2}}{\binom{A}{a}\binom{a}{2}} \sum_{i_1 < i_2 < \dots < i_a}^A \tilde{V}_{i_1 i_2 \dots i_a} , \quad (4)$$

with

$$\tilde{V}_{12\dots a} = e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} - \sum_{i=1}^a h_i , \quad (5)$$

and $S^{(a)}$ is an a -body operator; $H_a^\Omega = h_1 + h_2 + h_3 + \dots + h_a + V_a$, and $V_a = \sum_{i < j}^a V_{ij}$. Note that there is no sum over “ a ” in Eq. (4) so there is no coupling between clusters in this approach. Also, we adopt the HO basis states that are eigenstates of the one-body Hamiltonian $\sum_{i=1}^A h_i$.

If the full Hilbert space is divided into a finite model space (“P-space”) and a complementary infinite space (“Q-space”), using the projectors P and Q with $P + Q = 1$, it is possible to determine the transformation operator S_a from the decoupling condition

$$Q_a e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} P_a = 0 , \quad (6)$$

and the simultaneous restrictions $P_a S^{(a)} P_a = Q_a S^{(a)} Q_a = 0$. Note that a -nucleon-state projectors (P_a, Q_a) appear in Eq. (6). Their definitions follow from the definitions of the A -nucleon projectors P, Q . The unitary transformation and decoupling condition, introduced by Suzuki and Okamoto and referred to as the unitary-model-operator approach (UMOA) [24], has a solution that can be expressed in the following form

$$S^{(a)} = \text{arctanh}(\omega - \omega^\dagger) , \quad (7)$$

with the operator ω satisfying $\omega = Q_a \omega P_a$, and solving its own decoupling equation,

$$Q_a e^{-\omega} H_a^\Omega e^{\omega} P_a = 0 . \quad (8)$$

Let us also note that $\bar{H}_{a\text{-eff}} = P_a e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} P_a$ leads to the relation

$$\bar{H}_{a\text{-eff}} = (P_a + \omega^\dagger \omega)^{-1/2} (P_a + P_a \omega^\dagger Q_a) H_a^\Omega (Q_a \omega P_a + P_a) (P_a + \omega^\dagger \omega)^{-1/2} . \quad (9)$$

Given the eigensolutions, $H_a^\Omega |k\rangle = E_k |k\rangle$, in the infinite Hilbert space for the cluster, then the operator ω can be determined from

$$\langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{k \in \mathcal{K}} \langle \alpha_Q | k \rangle \langle \tilde{k} | \alpha_P \rangle , \quad (10)$$

where we denote by tilde the inverted matrix of $\langle \alpha_P | k \rangle$, i.e., $\sum_{\alpha_P} \langle \tilde{k} | \alpha_P \rangle \langle \alpha_P | k' \rangle = \delta_{k,k'}$ and $\sum_k \langle \alpha'_P | \tilde{k} \rangle \langle k | \alpha_P \rangle = \delta_{\alpha'_P, \alpha_P}$, for $k, k' \in \mathcal{K}$. In the relation (10), $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ are the model-space and the Q-space basis states, respectively, and \mathcal{K} denotes a set of d_P eigenstates, whose properties are reproduced in the model space, with d_P equal to the dimension of the model space.

In practice, the exact (to numerical precision) solutions for the $a=2$ cluster are obtained in basis spaces of several hundred $\hbar\Omega$ in each relative motion NN channel.

We note that in the limit $a \rightarrow A$, we obtain the exact solutions for d_P states of the full problem for any finite basis space, with flexibility for the choice of physical states subject to certain conditions [25].

We define our P-space to consist of all A-particle configurations in the oscillator basis with oscillator energy less than or equal some cutoff value, $N_m = N_{min} + N_{max}$, where N is the sum of $2n+l$ values of the occupied single particle states in the configuration. N_{min} is the minimum value required by the Pauli principle and equals 84 for these $A = 48$ nuclei. Our P-spaces are equally described by the excitations allowed through N_{max} which begins with 0. The cluster space, P_2 , is defined by the range of 2-body states encountered in the P-space.

Due to our cluster approximation a dependence of our results on N_{max} and on $\hbar\Omega$ arises. For a fixed cluster size, the smaller the basis space, the larger the dependence on $\hbar\Omega$. The residual N_{max} and $\hbar\Omega$ dependences can be used to infer the uncertainty in our results arising from the neglect of effective many-body interactions.

In light nuclei, the strategy has been to evaluate H_{eff} for each model space leading to a separate H_{eff} for positive and negative parity states. As one proceeds to heavier systems we reason that a better strategy is to use the same H_{eff} for both positive and negative parities e.g. use the $1\hbar\Omega$ H_{eff} in both the $0\hbar\Omega$ and $1\hbar\Omega$ model spaces. The logic for the revised strategy stems from three considerations: (1) either strategy will converge to the exact result in sufficiently large basis spaces; (2) for adjoining spaces in heavier systems, the predominant sets of pairwise interactions are in the same configurations with just one pair at a time shifting to the larger space; and (3) for electromagnetic transitions between states of opposite parity, the theory of the corresponding effective operators will be simplified.

To elaborate on the second point, we note that the bulk of the binding should not be altered in proceeding from a $0\hbar\Omega$ to a $1\hbar\Omega$ model space in $A=48$, suggesting the same H_{eff} is preferred. For small model spaces, such as those investigated here, the revised strategy improves the splitting between positive and negative parity states for the physical reason just mentioned.

This revised strategy simplifies our work to evaluate H_{eff} since it is required only for every other increment in the basis space, such as $1\hbar\Omega$, $3\hbar\Omega$, $5\hbar\Omega$, etc., to evaluate the converging sequence.

In order to construct the operator ω (10) we need to select the set of eigenvectors \mathcal{K} . We select

the lowest states obtained in each two-body channel. It turns out that these states also have the largest overlap with the model space for the range of $\hbar\Omega$ we have investigated and the P-spaces we select.

We input the effective Hamiltonian, now consisting of a relative two-body operator and the pure H_{CM} term introduced earlier, into an m-scheme Lanczos diagonalization process to obtain the P-space eigenvalues and eigenvectors [26]. At this stage we also add the term H_{CM} again with a large positive coefficient to separate the physically interesting states with $0s$ CM motion from those with excited CM motion. We retain only the eigenstates with pure $0s$ CM motion when evaluating observables. All observables that are expressible as functions of relative coordinates, such as the rms radius and radial densities, are then evaluated free of CM motion effects.

In the case of the $0\hbar\Omega$ model space for ^{48}Ca , the neutrons occupy part of the pf shell while the protons fill the sd shell. Now, for the $1\hbar\Omega$ model space that we adopt for ^{48}Ca , we take proton pairs in the Q-space as those with relative harmonic oscillator states having $(2n+l) \geq 6$. Similarly, we take neutron pairs in the $1\hbar\Omega$ Q-space having $(2n+l) \geq 8$. For the neutron-proton pairs we take the Heff with pairs in the Q-space of $(2n+l) \geq 7$. This defines the effective Hamiltonian for both positive and negative parity states.

It is important to note that we retain this same Hamiltonian for all the $A = 48$ results presented here even though some have protons in the pf shell. In so doing, we recognize that these are additional approximations that we expect to become less severe in future efforts with enlarged P-spaces.

Since we have chosen separate P-spaces for the neutrons and the protons, we felt the need to confirm that our treatment of the spurious CM motion remains valid. We tested this with the ^{48}Ca positive parity spectrum in the following way. We lowered the Lagrange multiplier of the H_{CM} term from our conventional value of 10.0 to a value of 2.0. In the past this was more than sufficient to reveal any deficiencies in our treatment of CM motion. In the present case this means that, since $\hbar\Omega = 10\text{MeV}$, our lowest spurious states are around 20 MeV of excitation in ^{48}Ca (assuming the CM motion is treated correctly). This is about as low as we can safely go for a test since we still have significant separation of the spurious from the non-spurious states.

The test showed that six of the lowest 15 eigenvalues changed by 1 keV, a change in the 6th significant figure, while the other 9 were unchanged at this precision, indicating at most a change in the 7th significant figure. This numerically demonstrates that the CM motion in the NCSM is accurately treated by the constraint method even when neutrons and protons occupy different shells, as long as the model space is defined with a many-body cutoff as we have implemented.

The m-scheme basis dimensionalities are (12022, 139046, and 634744) for (^{48}Ca , ^{48}Sc , and ^{48}Ti) respectively in the $0\hbar\Omega$ model spaces, and 2921360 for ^{48}Ca in the $1\hbar\Omega$ model space. By way of

reference, ^{48}Ca in the $2\hbar\Omega$ model space produces an m-scheme matrix dimension of 214664244.

We close our outline on the theoretical framework with the observation that all observables require the same transformation as implemented on the Hamiltonian. To date, we have found rather small effects on the rms radius operator when we transformed it to a P-space effective rms operator at the $a=2$ cluster level [17]. On the other hand, substantial renormalization was observed for the kinetic energy operator when using the $a = 2$ transformation to evaluate its expectation value [27]. More recently, the underlying physics of effective operator renormalization has been explored in detail and major improvements in the short-range and/or high momentum transfer properties of nuclei have been found to be accurately treated by the theory [28].

It is especially noteworthy that our NCSM treatment in the full $0\hbar\Omega$ basis space exactly preserves the Ikeda sum rule [12]. We verified this by explicit calculations in our applications here.

B. Phenomenological adjustments

To obtain NCSM spectroscopies fit to the data for these $A = 48$ nuclei by means of additive phenomenological potentials is a major undertaking. Hence, we investigate here minimal approaches to modifying the theoretical Heff to improve selected spectroscopic properties. We consider this as a baseline effort for future investigations in larger model spaces where we believe there will be a reduced need for phenomenological terms.

Our overall fitting strategy is to emphasize the total binding energy and the lowest lying excited states.

Inspired by successful modifications found in Ref. [7], we first investigated whether a phenomenological S-wave or monopole interaction supplies the main missing ingredient from our NCSM realistic effective two-body Hamiltonians. We chose to add simple $T = 0$ and $T = 1$ delta functions and we found that they can produce greatly improved properties. However, we find it necessary to adjust the $T = 0$ and $T = 1$ strengths for each nucleus to obtain the good agreement with experimental properties. Thus, we conclude that, with this approach, six parameters are needed to obtain reasonable results for the binding energies and the positive parity spectra of the three nuclei we address. However, the spectrum of ^{48}Sc is still rather poor.

The recent review of the phenomenological shell model and the role of the monopole interaction [9] demonstrates that the ultimate source of the residual physics we will need is contained in 3-body interaction effects - probably a combination of core-polarization and realistic (bare) 3-body forces. Our long term goal is to include these additional contributions which are natural in our NCSM approach but require next-generation computers. In order to appreciate the magnitude of the effort needed and the potential success of including realistic NN and NNN interactions in large

basis spaces, we refer the reader to the recent investigation of ${}^7\text{Li}$ with a Hamiltonian derived from chiral effective field theory [29].

In addition, more detailed examination of the features of our results (see below) and comparisons with NCSM results in light nuclei indeed indicate the missing physics is tied to larger basis spaces and to realistic NNN interactions. The fact that a simple monopole term in the conventional shell model with a core successfully approximates all this complexity at the 2-body level is remarkable and deserves more extensive investigation.

In the hopes of obtaining a single NCSM Hamiltonian for the binding energies and spectra of these three nuclei, we then explored the utility of two-body central plus tensor forces added to the ab-initio H_{eff} . We achieve a reasonable description of a small set of the targeted properties in these three nuclei by fitting the strengths and ranges of these three terms.

The specific forms of the finite range central and tensor potentials we found acceptable are as follows:

$$V(r) = V_0 \exp(-(r/R)^2)/r^2 + V_1 \exp(-(r/R)^2)/r^2 + V_t S_{12}/r^3 \quad (11)$$

where the central strengths, $V_0 = -14.40 \text{ MeV} - fm^2$ and $V_1 = -22.61 \text{ MeV} - fm^2$ with $R = 1.5 fm$, the tensor strength $V_t = -52.22 \text{ MeV} - fm^3$, and S_{12} is the conventional tensor operator.

III. RESULTS AND DISCUSSION

We begin with a survey of the ground state eigenenergies of $A = 48$ nuclei presented in Fig. 1. The experimental values and extrapolations based on systematics [30] are presented as square points and portray the valley of stability with ${}^{48}\text{Ti}$ being the most stable $A = 48$ system. The upper set of results (round dots) are those obtained with the ab-initio NCSM as outlined above with the CD-Bonn interaction [22] and $\hbar\Omega = 10 \text{ MeV}$, a typical choice for this region. Note that the trend of the even-even and odd-odd nuclear binding energies matches reasonably well with experiment except that theory consistently underbinds by about 20 MeV (0.4 MeV/nucleon). In other words, except for this underbinding, the ab-initio NCSM already predicts some subtle features of the valley of stability.

While all even-even nuclei obtained here in the ab-initio NCSM have the correct $J^\pi = 0^+$ ground state spin and parity, the odd-odd nuclei generally have the incorrect ground state spin.

The point proton (neutron) rms radii are 3.51, 3.55, and 3.59 fm (3.75, 3.73, and 3.71 fm) for ${}^{48}\text{Ca}$, ${}^{48}\text{Sc}$ and ${}^{48}\text{Ti}$ respectively, when evaluated with the bare operator in the intrinsic coordinate

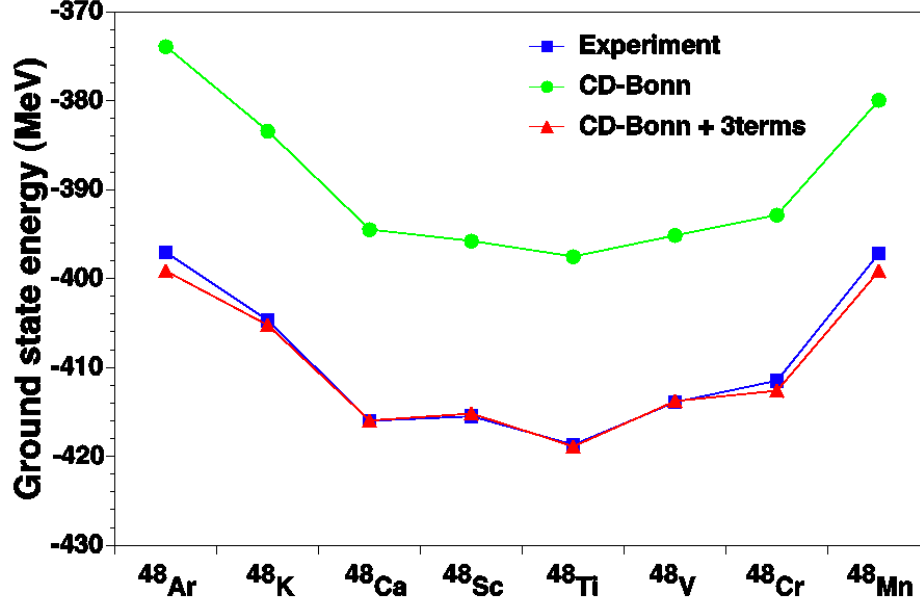


FIG. 1: (Color online) Ground state energies in MeV of $A = 48$ nuclei. At the extremes of the valley of stability, these energies are determined by systematics and the label "experiment" is to be understood in that context. The ab-initio NCSM results labelled "CD-Bonn" [22] are obtained with H_{eff} in the $1\hbar\Omega$ model space, $\hbar\Omega = 10 \text{ MeV}$ and isospin breaking in the P-space, as described in the text. The same H_{eff} with added gaussian central terms and a tensor force is used for the results labelled "CD-Bonn + 3 terms".

system. Of course, due to the limited model space, these results are insensitive to configuration mixing and are controlled by the choice of $\hbar\Omega$.

Increasing $\hbar\Omega$ leads to increased binding (and decreased rms radii) in this application of the ab-initio NCSM ($\hbar\Omega = 10.5 \text{ MeV}$ would produce a good fit to the binding alone) but fails to improve the errors in ground state spins and other deficiencies in the spectral properties described below in more detail.

The overall binding energy picture is considerably improved with the phenomenological additions described above. These additive terms were fit by hand to the ground state energies of ^{48}Ca , ^{48}Sc and ^{48}Ti as well as the first excited positive and negative parity states in ^{48}Ca . This limited amount of data under-constrains the fit and alternative parameterizations of the additive terms would yield equivalent fits to these limited data. Our approach here was to cease fitting when the first successful fit was obtained. Hence, all other properties of these $A = 48$ nuclei, including the ground state energies of the remaining 5 nuclei presented in Fig. 1, constitute predictions of this model. With the additive terms, the ground state spins and parities for the eight nuclei evaluated

now agree with experiment, where available.

We again stress that the ab-initio NCSM Hamiltonian and the fit Hamiltonians are pure 2-body Hamiltonians describing the interactions of all $A = 48$ nucleons. There is no division into valence and core subsystems, no explicit mean field and no single-particle energies. In addition, all results that we present are free of effects from spurious CM motion. We choose to distinguish the ab-initio NCSM from the model with additive phenomenological terms by referring to the latter as simply the "no-core shell model" or "NCSM" without the "ab-initio" adjective. For convenience in labelling figures and tables, we employ H_{eff} or "CD-Bonn" for the former and "CD-Bonn + 3 terms" for the latter.

Fig. 2 presents the $0\hbar\Omega$ model space results for ^{48}Ca with the CD-Bonn effective Hamiltonian, $[H_{eff}]$, at three values of the basis space parameter, $\hbar\Omega = 10$ (two cases), 11, and 12 MeV. The first column presents the experimental ground state and first two excited states. For $\hbar\Omega = 10$ MeV, we present results for the 1995 version of CD-Bonn (second column in the figure labelled "CDB") and for the 2000 version (third column labelled "CDB2K") [22] in order to display the minor differences in the spectra from these two potentials.

The main impression from Fig. 2 is that the spectra in ^{48}Ca are severely compressed relative to the experimental spreading. Inspecting the corresponding ground state wavefunctions reveals an absence of the expected dominance by the $[0f_{7/2}]^8$ neutron configuration. Instead, the $1p_{3/2}$ neutron state is significantly populated. We conclude that the expected energy spacing between the $0f_{7/2}$ and the $1p_{3/2}$ state is not supported by the ab-initio NCSM in such a small model space. This means there is insufficient spin-orbit splitting.

Here, we can remark that a recent mean-field study with similarly derived H_{eff} showed some deficiency in the spin-orbit splitting for ^{16}O in smaller model spaces when compared with experiment [31]. Similarly, a detailed study of ^{12}C neutrino scattering and magnetic transition observables revealed that the $a = 2$ cluster approximation underpredicts the spin-orbit splitting needed to explain these data [32]. This deficiency appears to be solved by the addition of true NNN forces and the use of larger basis spaces which are beyond the scope of our present efforts. Detailed investigations of the binding energies and spectroscopy of p-shell nuclei have also provided strong evidence of the need for true NNN forces when standard high-quality NN interactions, such as CD-Bonn or Argonne V18, are employed [33]. This need is manifest significantly in the spin-orbit properties.

We do not display the theoretical negative parity states in this case but we comment that they are similarly compressed relative to the experimental spreading. Furthermore, the lowest negative parity state appears at a rather high excitation energy. This feature is reminiscent of the results obtained for ^{12}C where the negative parity spectra appeared high relative to the positive parity

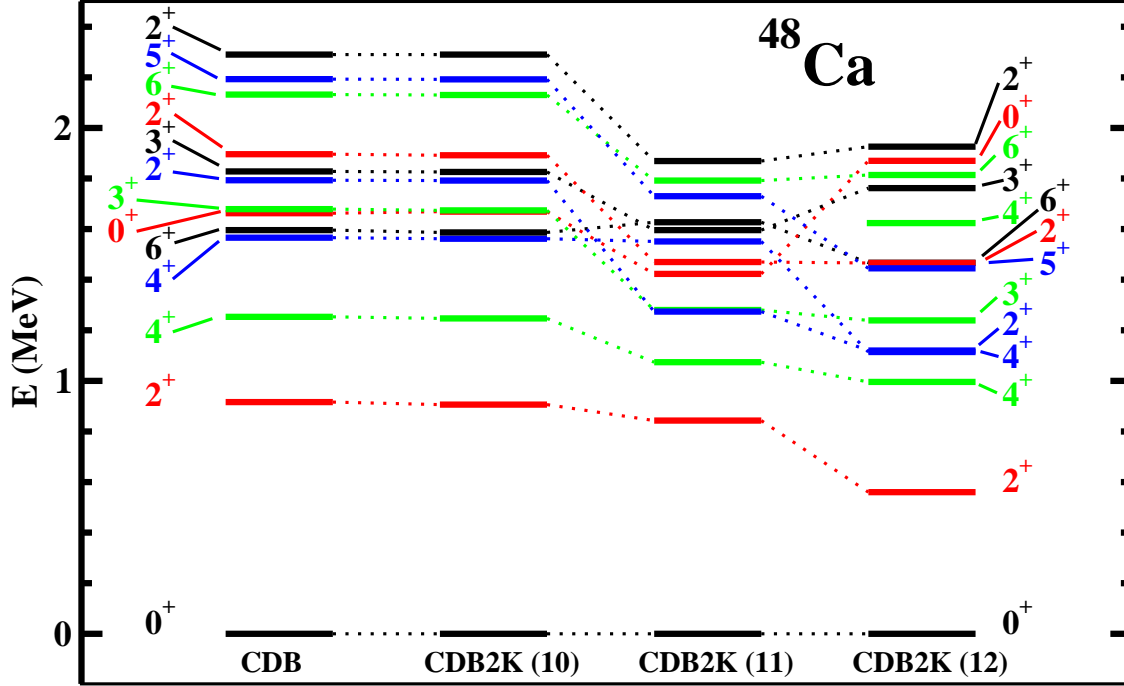


FIG. 2: (Color online) ^{48}Ca positive parity excitation spectra (in MeV) for the CD Bonn (1995) (column 1) effective Hamiltonian (labelled "CDB") and the CD Bonn (2000) (columns 2-4) effective Hamiltonian (labelled "CDB2K") in the $0\hbar\Omega$ harmonic oscillator basis space with $\hbar\Omega = 10, 11$, and 12 MeV as indicated by the number in parenthesis in each label. The experimental spectrum is not shown due to the absence of any experimental states below 3.8 MeV of excitation. CD-Bonn interactions are taken from Ref. [22]. Dotted lines connect nearby states of the same spin in ascending order.

spectra for model spaces up through $3\hbar\Omega$ [17].

Note, however, that when we adopt the new strategy discussed above, using the H_{eff} of the $1\hbar\Omega$ model space for both the positive and negative parity states at $\hbar\Omega = 10\text{MeV}$, the relative spacings of the states within a given parity are essentially unchanged while the lowest negative parity excitation above the ground state is now at 6.9 MeV of excitation, a major improvement. This will be discussed shortly along with other results in Fig. 3.

Figs. 3 - 5 display, in column 2 labelled "CDB + 3 terms", the spectra for these $A = 48$ nuclei resulting from our best fit Hamiltonian as described in the previous section. The resulting BE/A were presented in Fig. 1 for eight $A = 48$ nuclei with this same Hamiltonian.

In each of the Figs. 3 - 5, we display the experimental spectrum in column 1 and the results of Ref. [7] in column 3.

As seen in Fig. 3, our fit yields a good description of the low-lying positive and negative parity

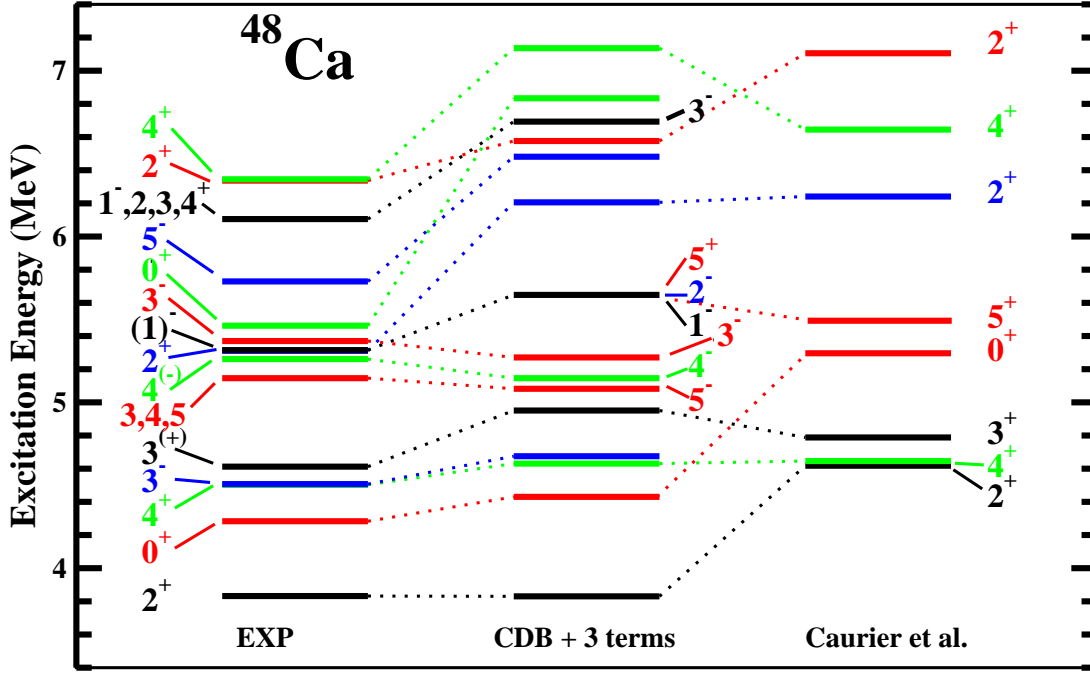


FIG. 3: (Color online) ^{48}Ca excitation spectra (in MeV) in the $\hbar\Omega = 10$ MeV harmonic oscillator basis for the NCSM effective Hamiltonian plus additive corrections (CDB + 3 terms) compared with experiment and with the results of [7] (Caurier, et al.). Positive and negative parity spectra are shown in the first two columns and the strength parameters are given in the text. Note that the 0^+ ground state is omitted from each spectrum and the theory spectra are shifted so that the ground states all coincide with the experimental ground state. Dotted lines connect nearby states that are likely to be related in character.

states of ^{48}Ca . In particular, we observe that the calculated first excited 0^+ , which was not involved in the fit, appears to be rather close to the experimental first excited 0^+ . On the other hand, we are missing another low-lying excited 0^+ . This may indicate that the intruder state inferred from the results presented in Ref. [7] is significantly mixed between the two low-lying excited 0^+ states in ^{48}Ca .

The reasonable agreement of our ^{48}Ca negative parity spectrum with experiment is significant considering that only the position of the first 3^- state was involved in our fit. It is also significant since the negative parity spectrum is sensitive to a set of 2-body matrix elements that is considerably larger than the set controlling the positive parity spectrum. In particular, we are sensitive to matrix elements involving excitations from the sd states to the pf states as well as from the pf states to the sdg states.

Turning now to ^{48}Sc shown in Fig. 4 we obtain one of the more important signatures of the success of the 3 term fit to these nuclei. Column 2 of Fig. 4 shows that we now obtain the correct ground state spin and a reasonable low-lying positive parity spectrum. Our spectrum is slightly more spread than the results of Caurier, et al., [7], but when comparing Fig. 3 and Fig. 4, please

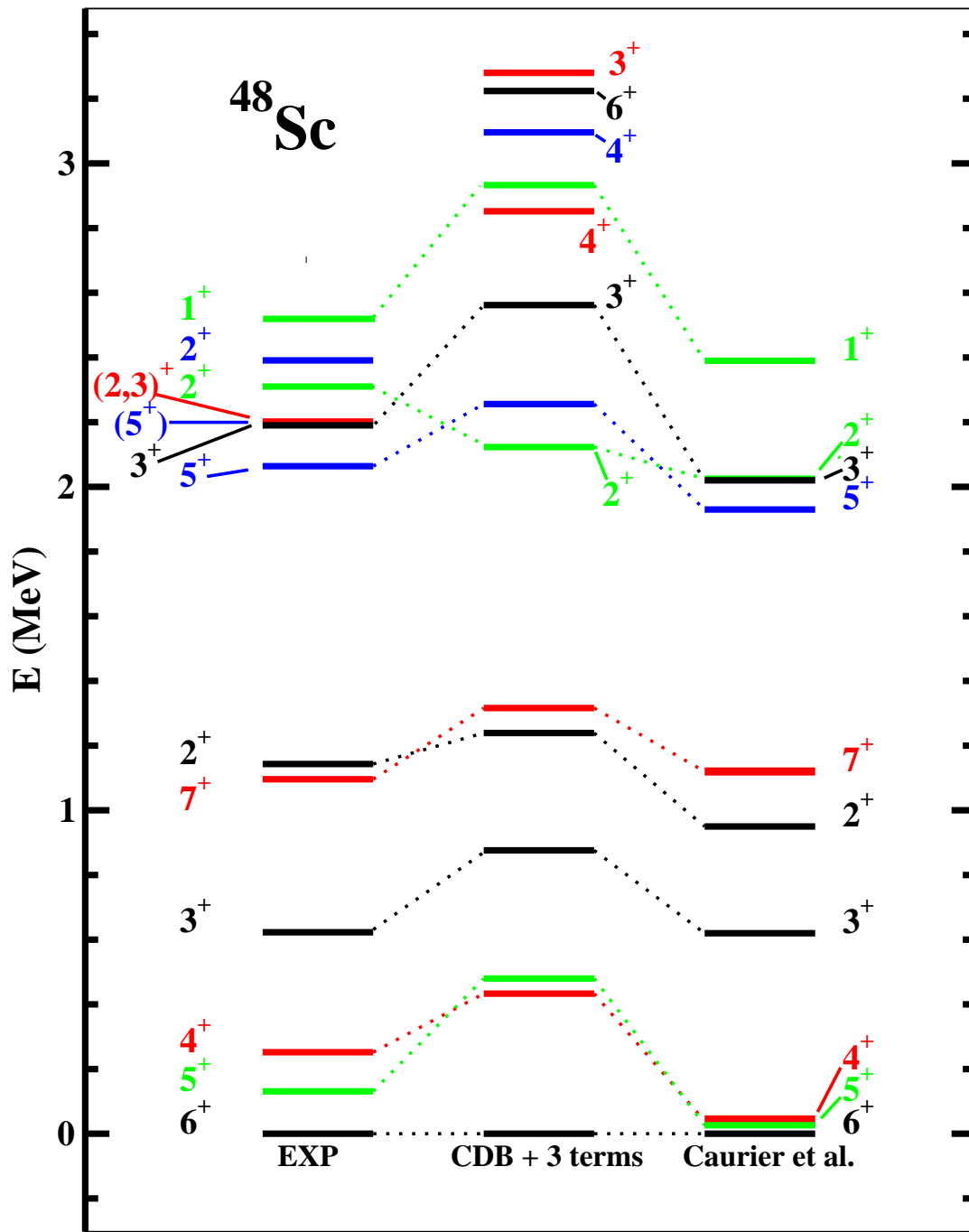


FIG. 4: (Color online) ^{48}Sc excitation spectra (in MeV) in the $\hbar\Omega = 10$ MeV harmonic oscillator basis for the NCSM effective Hamiltonian plus additive corrections (CDB + 3 terms) compared with experiment and with the results of [7] (Caurier, et al.). Dotted lines connect nearby states that are likely to be related in character.

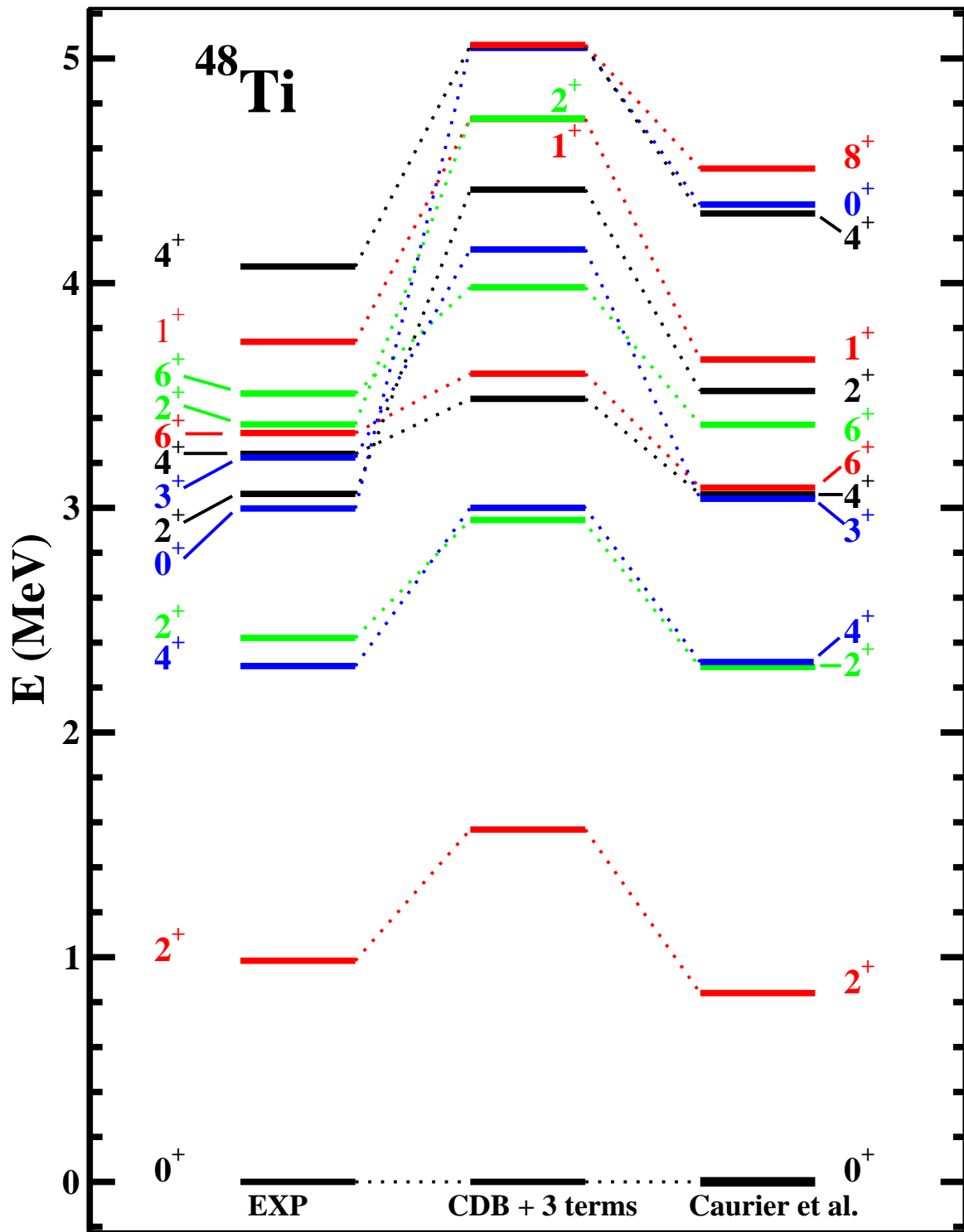


FIG. 5: (Color online) ^{48}Ti excitation spectra (in MeV) in the $\hbar\Omega = 10$ MeV harmonic oscillator basis for the NCSM effective Hamiltonian plus additive corrections (CDB + 3 terms) compared with experiment and with the results of [7] (Caurier, et al.). Dotted lines connect nearby states that are likely to be related in character.

note the greatly expanded scale in Fig. 4.

Our plan to apply these results for $\beta\beta$ processes, leads us to comment on the 1^+ states in ^{48}Sc . There are eight established 1^+ states below 5.1 MeV of excitation and our 3 term fit spectrum provides only five 1^+ states over the same span. Given our limited model space and the possibility of intruder states, we may expect additional states to appear when the model space is eventually enlarged. In the meantime, our beta transition strength function will be distributed over a more limited set of states in a way that will approximate the distribution among the more dense experimental spectrum of 1^+ states. Of course, we will include an even larger set of 1^+ states up to higher excitation energies when evaluating the double beta decay rate in a later effort.

Finally, we consider the case of ^{46}Ti shown in Fig. 5. Here again, the low-lying positive parity spectrum from CDB + 3 terms is in reasonable agreement with experiment except that it is more spread. We note one particular deficiency - the $0^+ - 2^+ - 4^+$ theoretical splitting is nearly that of a vibrator while the experimental spacings indicate a tendency toward rotational character. The fit of Caurier, et al., [7] succeeds better in this collective property. It will be interesting to discover whether the rotational character emerges from our model as we proceed further into the open shell situation.

We summarize the comparison between our theoretical spectra and the experimental spectra for three nuclei involved in the fit in Table I. The rms energy deviations between theory and experiment (excluding states involved in the fit) indicate that there is considerable room for improvement in the spectrum of ^{48}Ti and that future fits should include a representative excited state from this spectrum.

IV. CONCLUSIONS AND OUTLOOK

Our main goals have been to present the first NCSM results for ^{48}Ca , ^{48}Sc and ^{48}Ti with effective Hamiltonians derived directly from a realistic NN interaction and to investigate phenomenological improvements. The ab-initio results display the shortcomings of the limited model spaces presently available as well as possible shortcomings from neglecting three-body forces. We answer the question of whether the NCSM can be adjusted to obtain reasonable fits with additive phenomenological two-body potentials in the affirmative. In particular, we show that additive isospin-dependent central terms plus a tensor force can achieve accurate BE/A and reasonable spectra for these three systems. In addition, accurate BE/A are obtained for eight $A = 48$ nuclei reproducing the experimental valley of stability. The net change of interaction energies is of the order of a few percent with the added phenomenological terms. More extensive searching could undoubtedly improve the fits to the low-lying spectra.

Future efforts motivated by the present results are many-fold. We intend to improve the ab-initio H_{eff} by extensions to the three-body cluster approximation and to include three-nucleon interactions. We foresee initial applications to $\beta\beta$ decay, both the $\nu\nu$ and 0ν decay channels, by first extending our calculations to the Gamow-Teller (+/-) strengths. In the near future, we will be able to address significantly larger basis states as well. As a first step, we explicitly calculated the Ikeda sum rule and found that it is obeyed exactly in the NCSM.

These future efforts represent major undertakings and depend on major increases in computational resources. We firmly believe these planned endeavors are warranted in light of the importance of retaining as much predictive power as possible when addressing $\beta\beta$ decay.

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Nucleus/property	J^π	Exp	CDBonn + 3 terms
$^{48}\text{Ca} : BE$ [MeV]	0^+	415.991	415.948*
E_{ex} [MeV]	2^+	3.832	3.830*
	0^+	4.283	4.430
	4^+	4.503	4.631
	3^-	4.675*	4.675*
	$3^{(+)}$	4.612	4.951 [3^+]
	3, 4, 5	5.146	5.082 [5^-]
	$4^{(-)}$	5.261	5.146 [4^-]
	2^+	5.311	6.206
	$(1)^-$	5.325	5.648 [1^-]
	3^-	5.370	5.271
$rms(Exp - Th)$ [MeV]	-	-	0.368
$^{48}\text{Sc} : BE$ [MeV]	6^+	415.490	415.182*
E_{ex} [MeV]	5^+	0.131	0.480
	4^+	0.252	0.433
	3^+	0.623	0.876
	7^+	1.096	1.316
	2^+	1.143	1.239
	5^+	2.064	2.256
	3^+	2.190	2.562
	2^+	2.276	2.123
	1^+	2.517	2.933
$rms(Exp - Th)$ [MeV]	-	-	0.268
$^{48}\text{Ti} : BE$ [MeV]	0^+	418.699	418.882*
E_{ex} [MeV]	2^+	0.984	1.568
	4^+	2.296	3.000
	2^+	2.421	2.946
	0^+	2.997	5.047
	2^+	3.062	4.416
	3^+	3.224	4.150
	4^+	3.240	3.485
	6^+	3.333	3.597
$rms(Exp - Th)$ [MeV]	-	-	1.008
Energy rms (3 nuclei) [MeV]	-	-	0.628

TABLE I: Binding energies and excitation energies of three nuclei from experiment and theory. The states indicated with the asterisk are used in the fit that determines the parameters of the three additive terms to the CDBonn effective Hamiltonian. The rms deviations between experiment and theory are quoted for the listed excited state energies whose spin-parity assignments are reasonably well-established and that are not used in the fitting procedure (8-9 states for each nucleus). Spin-parity assignments used to relate theory with experiment, when the experimental assignments are uncertain, are indicated in square brackets next to the theoretical state. The overall energy rms for a total of 25 excited states is quoted at the end of the table.